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Functional integrals for Hartree–Fock–Bogoliubov many-body matrix elements

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Abstract

We discuss exact functional integral expressions for many-body matrix elements of the type $\langle\psi, A|e^{-\beta\hat{H}}|\psi, A\rangle$, between particle number projected Hartree–Fock–Bogoliubov (HFB) wavefunctions with time-reversal symmetry. A proof of positivity is given for a class of Hamiltonians and when the HFB wavefunctions with time-reversal symmetry are particle number projected to an even number of particles. We show explicitly how to reduce the propagator in the functional integral to a Hermitian positive definite propagator for particle pairs. This result generalizes that previously obtained using Bardeen–Cooper–Schrieffer wavefunctions.

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1. Introduction

Using the knowledge of many-body matrix elements of the type

$$\mathcal{B} = \langle\psi, N, Z|e^{-\beta\hat{H}}|\psi, N, Z\rangle \tag{1}$$

where $\hat{H}$ is the many-body Hamiltonian of N and Z interacting neutrons and protons and $|\psi, N, Z\rangle$ is an input many-particle state having particle number N, Z, in the limit of large β, we can calculate ground-state properties.

Recently, a functional integral formalism, which gives expressions for the above matrix elements, has been introduced in the context of Monte Carlo calculations, for the pairing plus quadrupole model [1] using functional integrals containing pairing fields. This formalism is sufficiently general to allow the calculation of a broad class of wavefunctions, namely wavefunctions which are exponentials of linear forms in pair creation operators.

In [2] it was shown that the integrand in the functional integral obtained in the density decomposition for the pairing plus quadrupole model is always positive for an even number of particles, provided that the input state $|\psi\rangle$ is a Slater determinant with time-reversal symmetry. An obvious limitation of the proof of [2] is that the best known approximation to the nuclear

wavefunction is the Hartree–Fock–Bogoliubov (HFB) approximation, rather than the Hartree–Fock (HF) approximation. Besides, the analysis of [2] is limited to Slater determinants, and it cannot be used for trial wavefunctions with built-in pairing correlations, such as HFB wavefunctions.

The purpose of this paper is precisely to remove such a limitation.

In [3], as an application of the formalism of [1], we have shown that if the input state $|\psi\rangle$ is of the Bardeen–Cooper–Schrieffer (BCS) type, which has exact angular momentum and parity 0^+, the functional integral with the same density decomposition used in [2] can be rewritten in terms of a Hermitian positive definite evolution operator for particle pairs and, of course, it is positive.

Here we apply the methods of [1] in order to extend the proof of [3] to the more general case for the input wavefunction, that is, any particle number projected quasi-particle vacuum with time-reversal symmetry. The resulting functional integral is positive definite and the propagator is still Hermitian positive definite and it refers to particle pairs as in [3]. We also discuss, as a particular case, Slater determinants, and again we show that the above result still holds. We give detailed proofs of the above statements.

These proofs are a consequence of the methods introduced in [1] but, rather than simply selecting the relevant cases out of the general formulae of [1, 3], it is just as economical to redo the derivation done in [1, 3] in the special case of the density decomposition for complex wavefunctions. Since nowhere in [1, 3] was the concept of quasi-particles used, we also rephrase the standard HFB wavefunctions using only particle concepts, rather than quasi-particles. The functional integrals we obtain for the matrix elements of equation (1) are new. In the following sections, we recall the class of Hamiltonians, and we discuss the functional integral, the type of wavefunction and finally we give the proof.

2. The class of Hamiltonians, the functional integral and the trial HFB wavefunctions

We consider only one particle species with Hamiltonian

$$\hat{H} = \hat{H}_0 - \sum_a \frac{k_a}{2} \hat{Q}_a^2 \tag{2}$$

where $\hat{H}_0 = \sum_{ij} a_i^\dagger (h_0)_{ij} a_j$ is the one-body term, and the two-body potential is written as a sum of squares with strength $k_a > 0$. $\hat{Q}_a$ (not necessarily, or not just the quadrupole operators) are one-body operators, i.e. in the notation of second quantization, $\hat{Q}_a = \sum_{r,s} (q_a)_{rs} a_r^\dagger a_s$. The pairing plus quadrupole Hamiltonian can be rewritten in this form with the pairing interaction written as $-G/2 \sum_{ij>0} \left[\left(a_i^\dagger a_j + a_{\bar{i}}^\dagger a_{\bar{j}} \right)^2 - \hat{N} \right]$, where $\hat{N}$ is the particle number operator and the state $\bar{i}$ is the time-reversal partner of the state i. The single-particle space is separated into two subspaces h_+ and h_-. The states belonging to h_+ have quantum numbers $nljm$ with the m values differing from each other by two units. The states belonging to h_- are the time-reversal partners of the states in h_+ and these are related to the states in h_+ by the relation $|\overline{nljm}\rangle = (-1)^{j+1/2} |nlj - m\rangle$. The notation $i > 0$ means that the state i belongs to h_+. The time-reversal operator changes the states in h_+ into the states in h_- and the states in h_- into the opposite of the states in h_+.

Unless stated otherwise, matrix indices run first over the h_+ states and then over the h_- states.

On this basis, the matrices h_0 and q_a have the following form,

$$\begin{pmatrix} r & s \\ -s^\star & r^\star \end{pmatrix} \tag{3}$$

where each of the submatrices r, s, $-s^\star$ and $r^\star$ represents the matrix elements between the single-particle states (i, j) , $(i, \bar{j})$, $(\bar{i}, j)$ and $(\bar{i}, \bar{j})$, respectively. The number of single-particle states forming the basis is denoted by N_s.

We consider Hamiltonians written in the separable form of equation (2), for which the single-particle matrix elements are in the form (3). This class of Hamiltonians was considered in [2], for which a proof of positivity of the functional integral was given.

The functional integral expression for $\mathrm{e}^{-\beta\hat{H}}$ is given by [4]

$$\mathrm{e}^{-\beta\hat{H}} = \mathrm{e}^{-\beta G\hat{N}/2}\mathcal{N}\int\prod_{n=1}^{N_t}\prod_a \mathrm{d}\sigma_{an}\,\mathrm{e}^{-\frac{\epsilon}{2}\sum_{an}k_a\sigma_{an}^2}\hat{U} \tag{4}$$

where $\hat{U}$ is the second quantized imaginary time propagator

$$\hat{U} = \hat{U}_{N_t}\hat{U}_{N_t-1}...\hat{U}_1 \tag{5}$$

with

$$\hat{U}_n = \mathrm{e}^{-\epsilon[\hat{H}_0-\sum_a k_a\sigma_{an}\hat{Q}_a]} \qquad n = 1, \ldots, N_t. \tag{6}$$

$\mathcal{N}$ is the normalization constant

$$\mathcal{N} = \prod_a\left(\frac{\epsilon k_a}{2\pi}\right)^{\frac{N_t}{2}}. \tag{7}$$

N_t is the number of time intervals and $\epsilon = \beta/N_t$. Equation (4) becomes exact in the limit $\epsilon \to 0$. The functional integral of equations (4)–(6) differs from the functional integral used in [1], which was written in terms of pairing fields and does not conserve the number of particles. The technique used in [1] nonetheless also applies to this functional integral in a straightforward way, which is discussed below.

We denote second quantized operators by capitals with a hat symbol and their corresponding first quantized operators by small letters, for example $\hat{Q}_a = \sum_{rs}(q_a)_{rs}a_r^\dagger a_s$.

Inserting equation (4) into equation (1), for A particles we have

$$\mathcal{B} = \mathrm{e}^{-\beta GA/2}\mathcal{N}\int\prod_{n=1}^{N_t}\prod_a \mathrm{d}\sigma_{an}\,\mathrm{e}^{-\frac{\epsilon}{2}\sum_{an}k_a\sigma_{an}^2}\langle\psi, A|\hat{U}|\psi, A\rangle. \tag{8}$$

This equation is sometimes called the functional integral in the density decomposition [2], since only terms such as $a_r^\dagger a_s$ appear in equations (5) and (6). Having selected the type of functional integral, we have to evaluate the following matrix elements:

$$\mathcal{M} = \langle\psi, A|\hat{U}|\psi, A\rangle. \tag{9}$$

As input wavefunctions for an even system, we consider

$$|\psi\rangle = \hat{V}|0\rangle \tag{10}$$

with

$$\hat{V} = \exp\left[\frac{1}{2}(a^\dagger\, a)\begin{pmatrix}R_{11} & R_{12}\\ R_{21} & R_{22}\end{pmatrix}\begin{pmatrix}a\\ a^\dagger\end{pmatrix}\right] \tag{11}$$

where we have used a matrix notation, and $(a^\dagger, a)$ is a row vector composed of all creation and all annihilation operators. The matrices R_{ij} $(i, j = 1, 2)$, general for the time being, must satisfy the relations $R_{22} = -\tilde{R}_{11}$ and $\tilde{R}_{ij} = -R_{ij}$ $(i \neq j = 1, 2)$ and are of dimension N_s. The state $|\psi\rangle$ in equation (10) does not have a definite number of particles and therefore will be particle number projected in order to be used in equation (9).

This state is usually interpreted as the vacuum for the following quasi-particle operators

$$b_i = \hat{V} a_i \hat{V}^{-1} \qquad i = 1, \ldots, N_s \tag{12}$$

since they satisfy the relation $b_i|\psi\rangle = 0$. The quasi-particle creation operators are defined as

$$\bar{b}_i = \hat{V} a_i^\dagger \hat{V}^{-1} \qquad i = 1, \ldots, N_s \tag{13}$$

and coincide with the ordinary creation operators if $\hat{V}$ is unitary. More directly, in matrix notation, the relation between the particle and quasi-particle operators is given by [5]

$$\begin{pmatrix} b \\ \bar{b} \end{pmatrix} = V \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \tag{14}$$

where

$$V = \exp \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \equiv \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}. \tag{15}$$

The dimensionality of V is $2N_s$. Equations (12)–(14) represent a way of moving particle creation and annihilation operators to the left or to the right of operators such as $\hat{V}$. The transformation V is now restricted, by the requirement of time-reversal symmetry, to have submatrices of the following form,

$$V_{i,j} = \begin{pmatrix} (V_{ij})_{rs} & (V_{ij})_{r\bar{s}} \\ -(V_{ij})^\star_{r\bar{s}} & (V_{ij})^\star_{rs} \end{pmatrix} \qquad i, j = 1, 2 \tag{16}$$

where V_{ij} has been explicitly written in terms of the submatrices in the (h_+, h_+), (h_+, h_-), (h_-, h_+), (h_-, h_-) subspaces, respectively.

As discussed in [5], any operator $\hat{V}$, as in equation (11), can be written as a product of three special transformations

$$\hat{V} = \hat{V}_c \hat{V}_0 \hat{V}_d \tag{17}$$

where $\hat{V}_c = \exp\left(\frac{1}{2} a^\dagger X a^\dagger\right)$, $\hat{V}_0 \propto \exp(a^\dagger T a)$ and $\hat{V}_d = \exp\left(\frac{1}{2} a Y a\right)$, provided V_{22} is nonsingular, with appropriate matrices X, Y and T. Inserting equation (17) into equation (10), apart from a normalization constant we obtain

$$|\psi\rangle = \mathrm{e}^{1/2 a^\dagger X a^\dagger}|0\rangle. \tag{18}$$

This state is invariant under time-reversal transformation. We can always consider nonsingular V_{22} and treat the case $\det V_{22} = 0$ as a limit of vanishingly small singular values of the matrix X.[1] The explicit expression of the antisymmetric matrix X in terms of the V_{ij} is

$$X = V_{12} V_{22}^{-1}. \tag{19}$$

Mathematically, the fact that equation (19) gives an antisymmetric matrix X follows from the relation

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tilde{V} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} V = 1 \tag{20}$$

valid for any matrix V of the type given in equation (15) for antisymmetric R_{12} and R_{21} and with $R_{11} = -\tilde{R}_{22}$.

Since all matrices R_{ij} in equation (15) have the structure of class (3) and since the product and the inverse of a matrix of class (3) belong to the same class, it follows that the matrix X

[1] The singular values $s_i \geqslant 0$ of a matrix M are defined by the relation $M = USU'$ where U and U' are unitary matrices and S is a diagonal matrix with non-negative entries s_i. The matrices U and U' diagonalize $MM^\dagger$ and $M^\dagger M$ respectively with eigenvalues s_i^2.

also belongs to class (3). According to a theorem of [6, 7], any arbitrary antisymmetric matrix X, of even dimensionality, can be written in the canonical form

$$X = \tilde{d}\begin{pmatrix} s & 0 \\ 0 & s \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} d \tag{21}$$

where d is unitary and s is diagonal (with dimensionality $N_s/2$) with non-negative diagonal entries s_i. The numbers $s_i, s_{\bar{i}}$ are the singular values of the matrix X and are pairwise degenerate. It easy to see that the unitary matrix d belongs to class (3). This is because d diagonalizes the Hermitian matrix $X^\dagger X$ which belongs to class (3) and which is known to be diagonalizable by a matrix of this class.

In order to see that the most general time-reversal HFB state is given by equation (18) for a generic matrix X, we have to show that this wavefunction can display a 'blocked structure' and a pairing structure [8]. To see this, we insert equation (21) into equation (18), then

$$|\psi\rangle = \mathrm{e}^{\sum_{i>0} c_i^\dagger s_i c_{\bar{i}}^\dagger}|0\rangle \tag{22}$$

where i and $\bar{i}$ ($i > 0$) refer to a pair of degenerate singular values. The new particle creation operators $c^\dagger$ in equation (22) are given, in matrix notation, by

$$c^\dagger = da^\dagger. \tag{23}$$

Therefore, expanding the exponential in equation (22)

$$|\psi\rangle = \prod_{i>0}\left(1 + s_i c_i^\dagger c_{\bar{i}}^\dagger\right)|0\rangle. \tag{24}$$

If some of the singular values s become very large, with s_b denoting these large singular values, apart from a normalization constant we have

$$|\psi\rangle = \left(\prod_{b>0} c_b^\dagger c_{\bar{b}}^\dagger\right)\prod\left(1 + s_i c_i^\dagger c_{\bar{i}}^\dagger\right)|0\rangle \tag{25}$$

which displays the blocked structure of the wavefunction. These consideration imply that any time-reversal HF or more general HFB state can be recast in the appealing form given by equation (18) without referring to quasi-particles. The form of equation (18) is the most economical way of writing the wavefunction of equation (10), since the redundancy in equation (10) is reduced to an overall scale factor[2] of the matrix X. If one considers unitary operators $\hat{V}$, $|\psi\rangle$ is still given by equation (18) with arbitrary X, that is, the constraint of unitarity for the matrix V does not imply any constraint for X. This can be seen by evaluating the matrix X, with equation (18), when the matrix V is unitary. In fact, the Bloch–Messiah decomposition for an arbitrary unitary matrix V of the type given in equation (15) (see [7, 8]) gives

$$V = \begin{pmatrix} d' & 0 \\ 0 & d'^\star \end{pmatrix}\begin{pmatrix} \bar{u} & \bar{v} \\ \bar{v} & \bar{u} \end{pmatrix}\begin{pmatrix} c' & 0 \\ 0 & c'^\star \end{pmatrix}.$$

Here c' and d' are arbitrary unitary matrices; the matrix $\bar{u}$ is diagonal with diagonal matrix elements $u_1, u_1, u_2, u_2, \ldots, 1, 1, \ldots$; and the matrix $\bar{v}$ is block diagonal of the form

$$\bar{v} = \begin{pmatrix} 0 & v_1 & & & & \\ -v_1 & 0 & & & & \\ & & 0 & v_2 & & \\ & & -v_2 & 0 & & \\ & & & & 0 & \\ & & & & & \ddots \end{pmatrix}$$

[2] We are only interested in the component of $|\psi\rangle$ that has A particles: $(a^\dagger X a^\dagger)^{A/2}|0\rangle$. Therefore the overall normalization of the wavefunction is the scale of the matrix X.

with $u_i^2 + v_i^2 = 1$. Here the basis is ordered as $1, \bar{1}, 2, \bar{2}, \ldots$ rather than $1, 2, \ldots, \bar{1}, \bar{2}, \ldots$. In the matrix $\bar{u}$ we have replaced entries with 0 with vanishing small u_k and in the matrix $\bar{v}$ we have replaced the unit diagonal matrix elements with the matrices $\begin{pmatrix} 0 & \sqrt{1-u_k^2} \\ -\sqrt{1-u_k^2} & 0 \end{pmatrix}$. A zero diagonal matrix element in $\bar{u}$ would generate an occupied ('blocked') single-particle state in the quasi-particle vacuum. But we can do just the same by considering vanishingly small positive u_k, since the limiting form of the quasi-particle vacuum is the same. There are an even number of these occupied single-particle states in the quasi-particle vacuum since we are considering an even nucleus. Using the Bloch–Messiah form for V and equation (19), we obtain equation (21), apart from renaming the rows and columns and provided we identify the singular values of X with v_k/u_k, without any condition on the matrix X.

Equation (18) is reminiscent of the Thouless theorem (see [8]), although the wavefunction that we have obtained is written in terms of particle operators and of the particle vacuum, rather than in terms of quasi-particle operators and the corresponding vacuum as in the Thouless theorem. Therefore, in the following, the concept of quasi-particles is no longer used.

To summarize, a HFB wavefunction can be defined quite generally as equation (18) with an unrestricted antisymmetric matrix X, for unitary or non-unitary transformations V.

To evaluate the matrix elements of equation (9) let us first introduce the operator

$$\hat{P} = \mathrm{e}^{\alpha \hat{N}} = z^{N_s/2} \exp\left[\frac{1}{2}(a^\dagger a)\begin{pmatrix} \alpha & 0 \\ 0 & -\alpha \end{pmatrix}\begin{pmatrix} a \\ a^\dagger \end{pmatrix}\right] \tag{26}$$

where $z = \mathrm{e}^\alpha$ is the fugacity and $\hat{N}$ is the particle number operator. Then we evaluate the fugacity-dependent matrix elements

$$\mathcal{M}'(z) = \langle 0|\hat{V}^\dagger \hat{P} \hat{U} \hat{V}|0\rangle \tag{27}$$

and finally isolate the coefficient of z^A in equation (27). Note that the operator $\hat{P}$ in equation (26) has been written in the form of equation (11). The evaluation of equation (27) and the construction of Hermitian positive definite propagators for particle pairs is done in next section.

3. Evaluation of $\mathcal{M}$ and construction of the pair propagator

We use the fundamental property of operators such as $\hat{V}$ in equation (11). In other words, to any operator $\hat{V}$, of the type of equation (11), there is a corresponding matrix V given by equation (15) and this correspondence preserves the multiplication; i.e. if $\hat{V}_3 = \hat{V}_2 \hat{V}_1$, then $V_3 = V_2 V_1$. Let us then rewrite the propagator $\hat{U}_n$ in the form of equation (11) as

$$\hat{U}_n = \hat{W}_n c_n \tag{28}$$

with

$$\hat{W}_n = \exp\left[\frac{1}{2}(a^\dagger, a)\begin{pmatrix} -\epsilon h_n & 0 \\ 0 & \epsilon \tilde{h}_n \end{pmatrix}\begin{pmatrix} a \\ a^\dagger \end{pmatrix}\right] \tag{29}$$

and

$$c_n = \mathrm{e}^{-\frac{\epsilon}{2}\mathrm{Tr}(h_n)} \qquad h_n = h_0 - \sum_a k_a \sigma_{an} q_a. \tag{30}$$

Therefore, the matrix corresponding to $\hat{W}_n$ is

$$W_n = \begin{pmatrix} W_{n11} & 0 \\ 0 & W_{n22} \end{pmatrix} \tag{31}$$

with

$$W_{n11} = \mathrm{e}^{-\epsilon[h_0 - \sum_a k_a \sigma_{an} q_a]} \tag{32}$$

and

$$W_{n22} = \mathrm{e}^{\epsilon[\tilde{h}_0 - \sum_a k_a \sigma_{an} \tilde{q}_a]}. \tag{33}$$

Thus, the evolution operator in equation (4) is

$$\hat{U} = c\hat{W} \qquad c = \prod_n c_n \qquad \hat{W} = \prod_n \hat{W}_n \tag{34}$$

and the matrix corresponding to $\hat{W}$ is

$$W = \begin{pmatrix} W_{11} & 0 \\ 0 & W_{22} \end{pmatrix} = \begin{pmatrix} \prod_n W_{n11} & 0 \\ 0 & \prod_n W_{n22} \end{pmatrix}. \tag{35}$$

In the above equations, the products are time-ordered; moreover we have

$$W_{22} = \tilde{W}_{11}^{-1}. \tag{36}$$

Finally, we use the result obtained in [5] concerning the vacuum expectation values of any operator of the type of equation (11)

$$\langle 0|\hat{V}|0\rangle = [\det(V_{22})]^{1/2} \tag{37}$$

where V_{22} is the $(2,2)$ submatrix of the matrix V corresponding to $\hat{V}$. Equation (27) then becomes

$$\mathcal{M}'(z) = z^{N_s/2} c \langle 0|\, \mathrm{e}^{-1/2 a X^\star a} \exp\left[\frac{1}{2}(a^\dagger, a)\begin{pmatrix} \alpha & 0 \\ 0 & -\alpha \end{pmatrix}\begin{pmatrix} a \\ a^\dagger \end{pmatrix}\right] \hat{W}\, \mathrm{e}^{1/2 a^\dagger X a^\dagger} |0\rangle. \tag{38}$$

The matrix W', which corresponds to the product of the operator in equation (38), is the product of the matrices which correspond to each factor. Therefore

$$\begin{aligned} W' &= \begin{pmatrix} 1 & 0 \\ -X^\star & 1 \end{pmatrix}\begin{pmatrix} z & 0 \\ 0 & 1/z \end{pmatrix}\begin{pmatrix} W_{11} & 0 \\ 0 & W_{22} \end{pmatrix}\begin{pmatrix} 1 & X \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} zW_{11} & zW_{11}X \\ -zX^\star W_{11} & \frac{1}{z}W_{22} - zX^\star W_{11} X \end{pmatrix}. \end{aligned} \tag{39}$$

Hence, equation (37) gives

$$\mathcal{M}'(z) = c z^{N_s/2}\left[\det\left(\frac{1}{z}W_{22} - zX^\star W_{11} X\right)\right]^{1/2}. \tag{40}$$

We can factor out the term $\frac{1}{z}W_{22}$ in the determinant of equation (40) and obtain

$$\mathcal{M}'(z) = c \det[W_{22}]^{1/2}\left[\det\left(1 - z^2 W_{22}^{-1} X^\star W_{11} X\right)\right]^{1/2}. \tag{41}$$

Finally, using the relation $\det W_{22} = \prod_n \det(W_n)_{22} = \exp[\epsilon \sum_n \mathrm{Tr}(h_n)] = c^{-2}$, with c defined by equations (34) and (30), and using equation (36), we have

$$\mathcal{M}'(z) = [\det(1 - z^2 \tilde{W}_{11} X^\star W_{11} X)]^{1/2}. \tag{42}$$

We now use the canonical representation of the matrix X of equation (21), and we use the fact that, for matrices of class (3), the following identity holds

$$\begin{pmatrix} r & s \\ -s^\star & r^\star \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} r & s \\ -s^\star & r^\star \end{pmatrix}^\star. \tag{43}$$

That is, we can move to the left or to the right of any matrix of class (3), the matrix $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, by taking the complex conjugate. Equation (42) then becomes

$$\mathcal{M}'(z) = [\det(1 + z^2 \mathcal{Y}^\dagger \mathcal{Y})]^{1/2} \tag{44}$$

where

$$\mathcal{Y} = \begin{pmatrix} \sqrt{s} & 0 \\ 0 & \sqrt{s} \end{pmatrix} d^\star W_{11} \tilde{d} \begin{pmatrix} \sqrt{s} & 0 \\ 0 & \sqrt{s} \end{pmatrix}. \tag{45}$$

In obtaining equation (45) we have used the matrix identity $\det(AB) = \det(BA)$. The matrix $\mathcal{Y}^\dagger \mathcal{Y}$ is Hermitian and positive definite and its eigenvalues, which we denote as $y_1^2 > y_2^2 > \cdots$, are the square of the singular values of the matrix $\mathcal{Y}$. Since $\mathcal{M}'(z)$ must be a polynomial in z^2, these eigenvalues must form degenerate pairs. Selecting one eigenvalue for each pair, we evaluate the square root of the determinant in equation (44) as

$$\mathcal{M}'(z) = \prod_i{}' \left[1 + z^2 y_i^2\right] \tag{46}$$

where the prime in the product means that only one eigenvalue appears for each degenerate pair. In equation (46) there is no additional sign associated with the square roots of the various determinants in equation (41). This is because (see [3]), since $\mathcal{M}'(z)$ must be a polynomial in z, it is a continuous function of z. Therefore, any additional sign associated with the square roots in equation (41) is independent of z. For $z = 0$ we have only vacuum matrix elements in equation (9), and therefore $\mathcal{M} = 1$; this is the same in equation (46). Therefore, the various roots in equation (41) do not introduce additional signs.

The coefficient of z^A in the product gives the desired value of $\mathcal{M}$ and it is obviously positive. At very low temperature, the dominant term is obtained by considering only the first $A/2$ eigenvalues and we obtain

$$\mathcal{M} = y_1^2 y_2^2 \ldots y_{A/2}^2. \tag{47}$$

These results generalize those obtained in [3], which correspond to the choice $d = 1$ in equation (21). The matrix $\mathcal{Y}^\dagger \mathcal{Y}$ is the propagator for particle pairs, while the propagator for particles is $\mathcal{Y}$. Its spectrum depends on the choice of the matrix X. Equation (46) is formally analogous to the fermionic partition function in the grand canonical ensemble of a gas of particles with energies $-2(\ln y_i)/\beta$, and each of these fermions is a particle pair. Although we always select HFB wavefunctions, the results are obviously valid even if no variational requirements are imposed in the choice of X.

If we consider the following choice for the singular values of X

$$s_1 = s_2 = \cdots = s_{A/2} \gg 1 \qquad s_{A/2+1} = s_{A/2+2} = \cdots = s_{N_s/2} = 0 \tag{48}$$

$|\psi\rangle$ becomes a Slater determinant for A particles (see equation (25)). Equation (46) (more precisely the coefficient of z^A in the expansion of the product) gives the matrix elements in equation (9) when the wavefunction is a Slater determinant. The choice of the matrix d in equation (21) then selects the particular Slater determinant, e.g. the self-consistent HF Slater determinant.

In the HFB approximation, both the singular values of X and the unitary matrix d are determined variationally, while only the latter is determined in the HF approximation. It is worth comparing the result for the matrix elements $\mathcal{M}$, just obtained, with the proof of positivity given in [2]. The main differences are the following. First of all, only Slater determinants were considered in [2] and the matrix elements were expressed as a positive determinant of a matrix of class (3); in such a case the eigenvalues of such a matrix appear in complex conjugate pairs. In our case instead, we obtain a Hermitian positive definite

matrix, which in some sense is the square of a propagator, and each eigenvalue represents the contribution of a pair to the matrix elements of equation (9). The eigenvalues that are relevant here are the eigenvalues of the pair propagator (see equation (46)), and these are the square of the singular values of the particle propagator. Moreover, our analysis is valid for any HFB wavefunction which is time-reversal invariant, with or without particle number projection. It should be noted that, usually, in functional integrals the propagators which appear in the integrand are of rather general type and they certainly do not have a Hermitian character; the formulations we have constructed instead have precisely such a feature. It should also be noted that this analysis reveals the physical meaning of the singular value decomposition of the propagators used in [2] for numerical stability in Monte Carlo calculations.

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